Final Report
High Resolution CFD and Modeling for Diesel Engine Simulation
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Introduction

This project focused on developing numerical methods for the simulation of large scale combustion processes. Our particular research focused on algorithm development for compressible flows, the development of geometric techniques fordealing with the complex geometries, and their application to problems of independent scientific research, for example the simulation of laser-induced spark ignited mixture. Our basic methodology used second order Godunov methods, which when used with limiters remain stable in the presence of discontinuities. We used block-structured adaptive mesh refinement (AMR) to enhance the local resolution only where needed. Much of our time was spent developing Cartesian embedded boundary methods for realistic engineer geometries. This is in contrast to body-fitted structured grids, where to handle the complexity many grids are needed, but each grid is logically rectangular. However Cartesian embedded grids introduce a layer of completely irregular cells at the boundary of the domain, with a less accurate representation of the solution than a body-fitted grid. Alternatively, we studied the use of immersed boundary methods for representing the evolution of material interfaces. These methods need special difference equations where the interface intersect the underling mesh.

Over the course of this grant, the PI and several postdocs were supported. Some of our research projects are summarized below. Much of it was in collaboration with colleagues at the DOE Laboratories (LBL, LLNL and Los Alamos) and at NASA Ames Research Center.

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Summary of Research

- **Robust Intersection of Multiple Component Geometries**
  We have developed an algorithm that takes multiple overlapping components and generates a single watertight description of the geometry. This greatly reduces the time it takes with a CAD program to prepare a surface description for mesh generation. The main technical difficulty in this work is overcoming the geometric degeneracies without paying the huge computational overhead typical of methods such as interval or exact arithmetic. To do this we use an adaptive precision floating point package, coupled with the SOS algorithm for perturbing the geometry into non-degenerate positions in a consistent way.

- **Cartesian Adaptive Mesh Generation**
  Using a variety of efficient algorithms and data structures, we have developed a new Cartesian mesh generator for embedded geometry that is capable of generating millions of cells a minute on a desktop workstation. It is the only such generator that handles split cells (Cartesian cells split into multiple regions by thin geometry), instead of relying on an often excessive use of mesh refinement to over-resolve thin geometry.
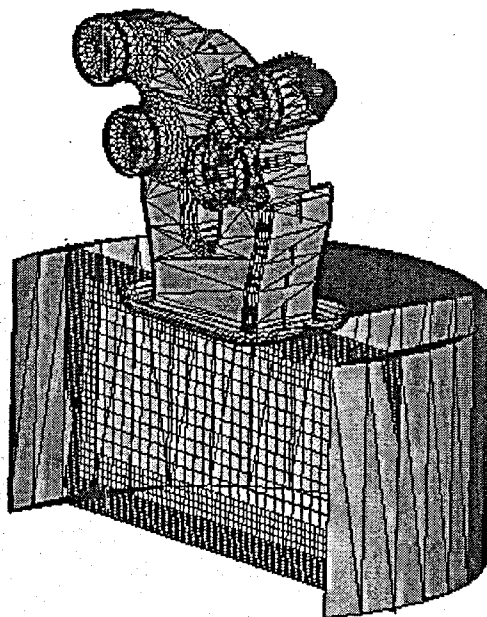

Figure 1: Diesel engine Cartesian embedded boundary mesh

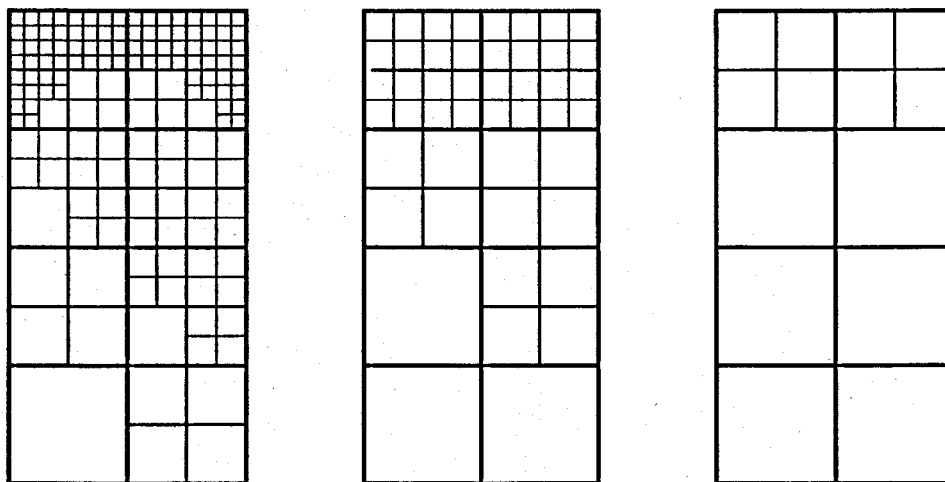## • Multigrid Mesh Generation for Embedded Boundary Grids

Figure 2: Two dimensional example of grid coarsening strategy.

We developed a multigrid strategy for accelerating convergence on these grids. Since we use unstructured grid data structure in the above work, we have a global grid covering the whole domain. This finest level grid contains cells of many different sizes. We use the Cartesian nesting of grids to generate the coarser level grids. A cell in the coarser level grid should be composed of the usual 8 fine cells in 3 dimensions, (or 4 cells in 2D), and is coarsened if all cells in fact appear in the finer grid. Figure 2 illustrates a sequence of grid levels in two dimensions. Experience with this strategy shows coarsening ratios of slightly better than 7 on reasonably sized fine meshes. One technical difficulty with mesh coarsening is recognizing split cells that can now be joined into one cut but not split coarse cell, or conversely, fine unsplit cells may coalesce into one coarse split cell (both of these can happen when coarsening the cut cells). A key issue of concern that still remains with multigrid on meshes with embedded geometry is whether or not the lack of resolution of the geometry (which is worse for non-body -fitted grids than the more common body-fitted variety) will impede convergence, or possibly reduce the number of grid levels that can be effectively used.

• Space-Filling Curves and Domain Decomposition

We developed an on-the-fly partitioning algorithm for parallel architectures based on space filling curves. Both the Morton ordering and the Peano-Hilbert orderings have previously been used in this context, but not for these kinds
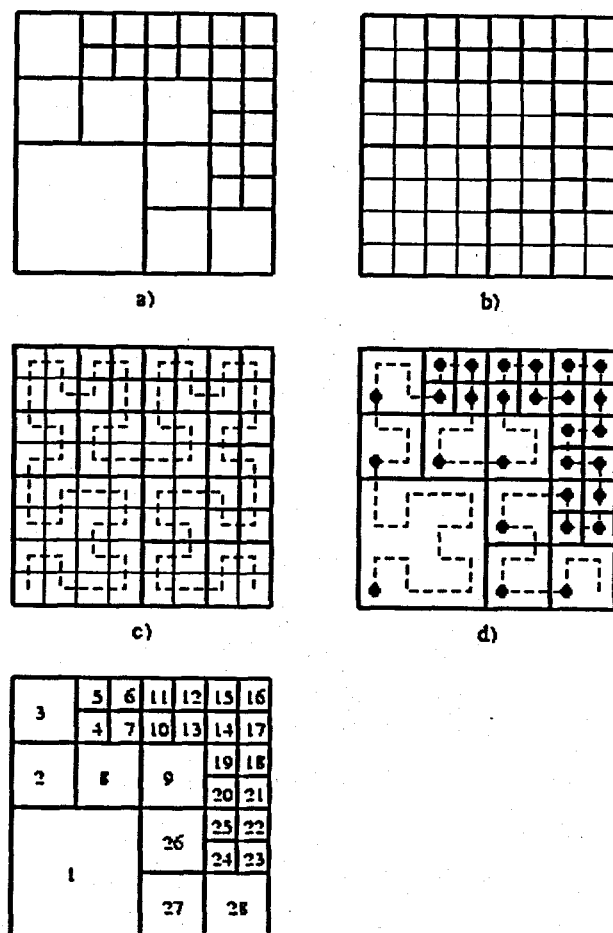
Figure 3: Example of space filling curve on multilevel mesh.

of grids or as a *dynamic* partitioning tool. It was a natural choice for Cartesian grids, where the partition cost is based on the number and types of cells (regular, cut, split) in the domain. It is simple to extend to the adaptive and anisotropic cases as well. Figure 3 illustrates the use of space filling curves on our grids.

- **Immersed Interfaces for Incompressible Two-Phase Flow with Surface Tension**
  We developed a numerical method to solving the incompressible Navier-Stokes equations for two phase flow with surface tension. For the description of the moving interface we used a level-set approach with reinitialization. The difficult, as with embedded boundaries above, is how to discretize in cells containing or adjacent to the interface. By including jump conditions for the pressure and its gradient across the interface, a system of equations in four unknowns (in two

4

dimensions) is derived and easily solved, preserving high resolution acorss the interface.

- **Cut Cell Boundary Conditions using the Full Cell Method**
  Since Cartesian embedded boundary grids leave cut cells with cell volumes that may be orders of magnitude smaller than a regular cell, it is a challenge to find stable and accurate boundary conditions for these cells with an explicit finite difference scheme. One of the simplest and most accurate approaches we developed to avoid the so-called *small-cell* problem (which however was not conservative) is to fill in the cut cells, and a set of ghost cells, so that cell updates are performed on regular grid cells. The fill-in is done using the nearest cell reflected across a solid boundary, with the sign of the normal velocity reversed. In effect a mirror flow is obtained by reflection. This is easily extended (at least in one dimension) so the case of moving bodies by incorporating a term for a reflecting wall moving at a given speed into the boundary condition.

- **UnderResolved Incompressible Flow Simulations**
  We studied the performance of difference approximations for the incompressible Navier Stokes equations when the computational mesh is underresolved. We demonstrated that all methods considered (a Godunov projection method, a primitive variable ENO method, an upwind vorticity stream-function method, and centered difference schemes, and a few others) produce spurious non-physical vortices. These artifacts appear to be due to a nonlinear effect in which the truncation error of the scheme initiates a vortex instability in the computed flow. The implication of this for the use of AMR is that grid refinement must be employed before large scale effects of underresolution have occurred, and that this must be accounted for in the criteria for automatically determining where a computational grid should be refined.